Critical Review of Henry's Law Constants and their Application to Environmental Regulations

J.C. Metsa
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T.N. Rogers and M.E. Mullins
Department of Chemical Engineering
Michigan Technological University
1400 Townsend Drive
Houghton, MI 49931, U.S.A.

E.J. Oman
Center for Clean Industrial Treatment Technology (CenCITT)
Michigan Technological University
1400 Townsend Drive
Houghton, MI 49931, U.S.A.

Experimental Henry's law constants compiled from AIChE DIPPR® (Design Institute for Physical Property Data) Project 911 and related work have been quantitatively tested for consistency via a variety of statistical methods (e.g., outlier checks, agreement between independent data sources, error evaluation of experimental methodologies, and trends within homologous series). These data values have also been examined for thermodynamic consistency, as defined by the Gibbs-Duhem equation, and then compared to predictions from a number of correlations and thermodynamic activity coefficient models. Chief among the data discrimination and validation tools are the group contribution models of UNIFAC and Hine-Mookerjee. The impact of the data variability on fate and treatment calculations, when used as inputs to EPA regulatory models, was also assessed.